

Hexamethylphosphoramide  
680-31-9 | DTXSID6020694

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 7.54e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 3.64e-01

Confidence level: 5.12e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Propene, 3,3,3-trifluoro-</div> <div>Measured: 4.60e-02</div> <div>Predicted: 3540</div>	<div>Image not found</div> <div>Cyclobutane, octafluoro-</div> <div>Measured: 1.10e-01</div> <div>Predicted: 3340</div>	<div>Image not found</div> <div>2-Pentene, 3-methyl-</div> <div>Measured: 4.69e-02</div> <div>Predicted: 156</div>
<div>Image not found</div> <div>2,3-Dimethylbutan-2-ol</div> <div>Measured: 12.0</div> <div>Predicted: 5.17</div>	<div>Image not found</div> <div>Fosthietan</div> <div>Measured: 5.13</div> <div>Predicted: 2.14e-05</div>	